

# Non-local quantum fluctuations and fermionic superfluidity in the attractive Hubbard model

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We study fermionic superfluidity in strongly anisotropic optical lattices with attractive interactions utilizing cluster DMFT and real-space DMFT methods and focusing in particular on the role of non-local quantum fluctuations. We show that non-local quantum fluctuations impact the BCS superfluid transition dramatically. Moreover, we show that exotic superfluid states with delicate order parameter structure, such as the Fulde-Ferrell-Larkin-Ovchinnikov phase driven by spin population imbalance, can emerge even in the presence of such strong fluctuations.

PACS numbers: 67.85.-d, 03.75.Ss, 71.10.Fd

Mean-field theories have been tremendously successful at furthering our understanding of quantum many-body physics. For instance, the explanation of conventional superconductivity based on the BCS-theory is hailed as one of the highest achievements in condensed matter physics. Nonetheless, it is well-known that the mean-field treatment in general can facilitate a qualitative description of the physical system – at best. In the context of lattice models, dynamical mean-field theory (DMFT) constitutes a substantial improvement over static mean-field treatments by including fully the effect of non-local quantum fluctuations. Yet, even the predictions of DMFT may fail in the presence of *non-local* quantum fluctuations, i.e. non-local contributions to the self-energy of the system. Ultimately, the emergence of an ordered phase can be firmly predicted only if the non-local quantum fluctuations are properly accounted for. Moreover, key information of the physical system can be encoded to the non-local structure of the self-energy. This is true for example for the d-wave symmetry of high temperature superconductors.

The elusive, yet ubiquitous, nature of non-local quantum fluctuations raises the question, whether it is possible to identify physical systems where the effects of these fluctuations could be studied in a systematic manner. In this respect, ultracold gas setups with controllable dimensionality seem to offer a natural path forward regarding that the non-local fluctuations are most prominent in low-dimensional systems. The dimensional crossover from 1D to higher dimensional systems has garnered broad interest. From the theoretical point of view, it is anticipated that phases of matter prominent in 1D models can be stabilized when brought to a higher dimensionality [1]. Experimentally, the strong dimensional anisotropy may also offer advantages over a more straightforward 3D geometry, as demonstrated in a recent work on repulsively interacting fermions in an anisotropic optical lattice, where the temperature scale of anti-ferromagnetic correlations was reached [2–4].

One of the most intriguing many-body phenomena

which can be approached in the context of dimensionally tunable lattices is that of fermionic superfluidity. The paradigm case of fermionic superfluidity with s-wave spin-singlet BCS pairing could be studied in an experimental realization of the attractively interacting Fermi-Hubbard model. Moreover, there is a wide consensus that this system might demonstrate exotic forms of superfluid pairing when subjected to e.g. a spin population imbalance. The prospects of realizing such forms of conventional and exotic superfluidity in systems of intermediate dimensionality have been discussed broadly in the literature [5–10]. However, the role of non-local quantum fluctuations remains to a large degree an open question in these systems even in the case of the conventional BCS pairing.

In this work, we study an attractively interacting two-component Fermi gas in a strongly anisotropic cubic optical lattice, see Fig. 1(a). We compute the phase diagram of this system using cluster and real-space variants of DMFT, and investigate the effect of non-local quantum fluctuations on the different possible forms of superfluidity occurring in the system.

The system is described by the Hubbard Hamiltonian

$$\begin{aligned} \mathcal{H} = & -t_{\parallel} \sum_{il\sigma} (c_{jl\sigma}^{\dagger} c_{(j+1)l\sigma} + \text{h.c.}) - t_{\perp} \sum_{\langle ll' \rangle} \sum_{i\sigma} c_{jl\sigma}^{\dagger} c_{j'l'\sigma} \\ & + U \sum_{jl} \hat{n}_{jl\uparrow} \hat{n}_{jl\downarrow} - \sum_{jl\sigma} \mu_{\sigma} \hat{n}_{jl\sigma}. \end{aligned} \quad (1)$$

Here, the index  $j$  is used to label the lattice sites within a single 1D chain, while the chains are labeled with the index  $l$ . The operator  $c_{jl\sigma}$  ( $c_{jl\sigma}^{\dagger}$ ) annihilates (creates) a fermion with pseudo-spin  $\sigma = \uparrow, \downarrow$  at site  $j$  in chain  $l$ . In the kinetic term,  $t_{\parallel}$  and  $t_{\perp}$  are the hoppings within the chain and between the chains, respectively, while the on-site interaction strength is denoted by  $U$  and the spin-dependent chemical potential by  $\mu_{\sigma}$ . In the following, we give all energies and temperatures in the units of  $t_{\parallel}$ , and set  $t_{\parallel} = 1$ . At  $t_{\perp} = 0$  the system is a collection of independent 1D chains whereas at  $t_{\perp} = 1$  we have a

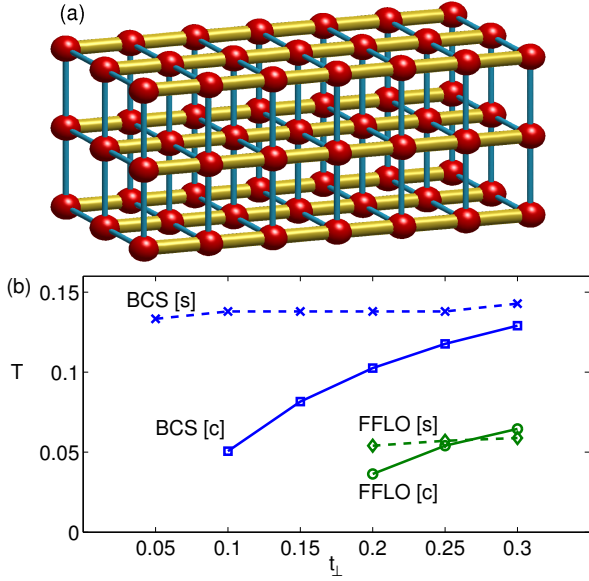


FIG. 1: (a) A schematic of the system geometry. The optical lattice consists of one-dimensional chains which are coupled to form an anisotropic cubic lattice. In our cluster DMFT scheme, the 1D chain is treated as a single cluster with periodic boundaries. (b) The BCS and FFLO phase transitions as a function of the interchain hopping  $t_{\perp}$  both in the cluster DMFT model (with non-local quantum fluctuations) and the real-space DMFT model (excluding non-local quantum fluctuations). The critical temperature of the BCS state is given by the continuous and dashed blue line for the cluster [c] and single-site [s] models, respectively. Similarly, the FFLO critical temperature is given by the green line for the cluster [c] model and by the dashed green line for the single-site [s] model. As a point of contrast, the static mean-field prediction of the BCS critical temperature is  $T_{c,\text{MF}} = 0.52$  in the corresponding parameter range, while the FFLO critical temperature would be on the order of  $0.5 T_{c,\text{MF}}$  [11]. In each case the system is at half-filling, and the FFLO transition is found by varying the spin-polarization of the system while maintaining the total filling fraction constant. For  $t_{\perp} \geq 0.15$ , we perform the calculations in a cluster of  $N_c = 36$  lattice sites, whereas for  $t_{\perp} = 0.1$  a cluster size of  $N_c = 42$  is required for convergence.

3D cubic lattice. The region  $0 < t_{\perp} < 1$  then defines a dimensional crossover from 1D to 3D. We study the system with an attractive interaction  $U = -3$ . Moreover, we describe the superfluid symmetry breaking using Nambu formalism. Thus, in the following equations, the Green's function and self-energy are interpreted in the form of  $2 \times 2$  Nambu blocks which are labeled by the position.

We solve the equilibrium state of the system using a cluster variant of dynamical mean-field theory (DMFT) [12, 13]. In our cluster DMFT model we assume a periodic boundary condition within a single chain and treat the whole chain as a single cluster in the algorithm. In the directions perpendicular to the 1D chains,

we assume that the self-energy of the system is local, i.e.

$$\Sigma_{jj';ll'}(i\omega_n) = \delta_{l,l'} \Sigma_{jj';l}(i\omega_n), \quad (2)$$

where  $i\omega_n$  is the Matsubara frequency. In other words, we take the self-energy as block diagonal in the interchain index  $l$ . On the assumption that the system is homogeneous in the interchain direction, the self-energy is independent of the chain index  $l$ , and moreover, the Green's function of the system is diagonal in the transverse quasi-momentum  $\mathbf{k}_{\perp} = (k_x, k_y)$ . The Dyson equation for the Green's function of the system is then given by

$$[\mathbf{G}(\mathbf{k}_{\perp}; i\omega_n)]_{jj'}^{-1} = [\mathbf{G}_{\parallel}^0(i\omega_n)]_{jj'}^{-1} - \epsilon_{\mathbf{k}_{\perp}} \sigma_z \delta_{jj'} - \Sigma_{jj'}(i\omega_n). \quad (3)$$

Here,  $\mathbf{G}_{\parallel}^0$  is the non-interacting Green's function of a single chain, while  $\epsilon_{\mathbf{k}_{\perp}}$  is the transverse single particle dispersion given by  $\epsilon_{\mathbf{k}_{\perp}} \equiv -2t_{\perp}(\cos k_x + \cos k_y)$  and  $\sigma_z$  the Pauli  $z$ -matrix. Taking a single chain as a cluster, the bath Green's function for the cluster DMFT becomes

$$[\mathcal{G}^0(i\omega_n)]_{jj'}^{-1} = \left[ \sum_{\mathbf{k}_{\perp}} \mathbf{G}(\mathbf{k}_{\perp}; i\omega_n) \right]_{jj'}^{-1} + \Sigma_{jj'}(i\omega_n). \quad (4)$$

We employ the continuous-time auxiliary-field quantum Monte Carlo method in Nambu formalism to solve the impurity problem of the DMFT iteration [14–16]. To facilitate the large expansion order imposed by the low temperature and the large cluster size of the simulations, we utilize delayed spin-flip update [17] and submatrix update [18] techniques to speed up the computation.

The construction of the cluster problem in the form of 1D chains as above is suitable for quasi-1D systems, and a similar approach has been utilized to study the Mott and Luttinger liquid transitions of the repulsive Hubbard model in quasi-1D lattices [19–21]. Moreover, our approach allows us to study the superfluid pairing on a general basis, including also the possibility of spatially non-uniform solutions. For example, in the presence of spin-polarization the two-component Fermi gas may enter the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) phase which involves spontaneous breaking of the translation invariance of the superfluid state [22, 23]. To give a point of contrast to alternative approaches, the cellular DMFT method could be criticized here for the explicit breaking of translation invariance on the level of the method, which might favor states with broken translation invariance. On the other hand, enforcing the spatial symmetry as in the dynamical cluster approximation (DCA) would contain precisely the opposite problem. Thus, we chose to adopt a periodic boundary condition which allows for solutions with broken translation invariance without introducing any such broken symmetry on the level of the computational method.

To provide a point of comparison for the cluster DMFT model we compute the phase diagram of the system using

single-site real-space DMFT [24–27], where the main assumption is that the self-energy is local. In this approximation, the expression for the self energy above simplifies further to  $\Sigma_{jj'}(i\omega_n) = \delta_{j,j'}\Sigma_j(i\omega_n)$ . Note that the self-energy is still frequency dependent, i.e. the model contains all local quantum fluctuations. The lattice Dyson equation remains in the same form as given in Eq. (3), while the quantum impurity model of DMFT is now reduced to a single site problem with a bath Green's function given by

$$[\mathcal{G}_j^0(i\omega_n)]^{-1} = \left[ \sum_{\mathbf{k}_\perp} \mathbf{G}_{jj}(\mathbf{k}_\perp; i\omega_n) \right]^{-1} + \Sigma_j(i\omega_n). \quad (5)$$

Notice that each matrix element above is still a  $2 \times 2$  Nambu block of the normal and anomalous on-site Green's functions or self-energies. Again, the reason for using the real-space formulation is that it allows us to describe also superfluid states with spatial symmetry breaking.

We define the superfluid order parameter as  $\Delta_j = -U\langle c_{j,\uparrow}^\dagger c_{j,\downarrow}^\dagger \rangle$ . Here, we identify the BCS state as the state with non-zero and uniform  $\Delta_j$  over the whole system. Since  $\Delta_j$  is defined as an anomalous expected value, this criterion also implies long range order. The FFLO state is defined as the state with  $\Delta_j$  oscillating with position. In order to study the FFLO mechanism we vary the spin-polarization  $P = (N_\uparrow - N_\downarrow)/(N_\uparrow + N_\downarrow)$  through the spin-dependent chemical potentials while keeping the total particle number constant at half-filling.

The phase diagram of the system is presented in Fig. 1(b). At  $t_\perp = 0.3$  the BCS critical temperature obtained from cluster DMFT is  $T_c = 0.13$  and decreases monotonously as the interchain hopping is reduced reaching a value of  $T_c = 0.05$  at  $t_\perp = 0.1$ . Below  $t_\perp = 0.1$ , we are limited by the computational cost of the impurity problem at cluster sizes and temperatures relevant for the BCS transition. However, the results for finite  $t_\perp$  suggest convergence to a critical temperature of zero at the 1D limit, as is expected because of the Mermin-Wagner theorem. To quantify the effect of the non-local quantum fluctuations on the BCS state, let us compare the result to the single-site DMFT calculations. The single-site DMFT predicts a nearly constant critical temperature for the BCS state with  $T_c \approx 0.14$  over the corresponding parameter range. It is then readily apparent that the rapid disappearance of superfluidity in the cluster model cannot be attributed to changes in the non-interacting density of states caused by the varying dimensionality. Such effects would already be included to the single-site model. Here, it should be noted that already the local quantum fluctuations bring a substantial correction the static mean-field prediction of the critical temperature  $T_{c,\text{MF}} = 0.52$ , though qualitatively the static mean-field and single-site DMFT critical temperatures behave similarly as a function of the interchain hopping.

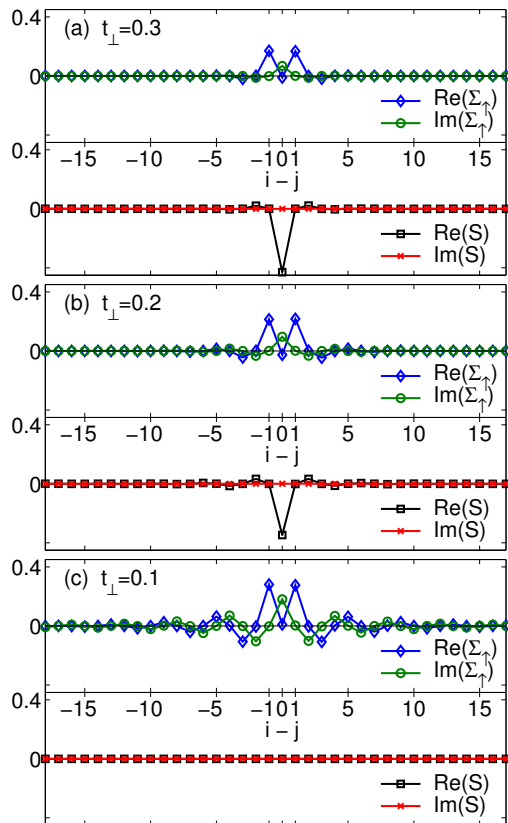


FIG. 2: The dependence of the self-energy on the dimensionality. In each panel we plot the normal spin- $\uparrow$  and anomalous Nambu components,  $\Sigma_{\uparrow,ij}(i\omega_n)$  and  $S_{ij}(i\omega_n)$ , of the self-energy between sites  $i$  and  $j$  for the lowest Matsubara frequency. Here, the system is at a temperature of  $T = 0.08$  and at half-filling with zero spin-polarization. At (a)  $t_\perp = 0.3$  and (b)  $t_\perp = 0.2$  this corresponds to the BCS state, while at (c)  $t_\perp = 0.1$  the system is in the normal phase. The non-local quantum fluctuations grow substantially as the interchain hopping  $t_\perp$  decreases. The oscillating structure of the self-energy in  $i-j$  is predominantly a single particle signature and corresponds to the Fermi momentum of the system.

In Fig. 2 we plot the self-energy of the system at a constant temperature while varying the interchain hopping  $t_\perp$ . The figure demonstrates that the non-local component of the self-energy grows rapidly towards the 1D limit. Therefore, we may conclude that the drastic decline of the superfluid critical temperature is driven by the non-local quantum fluctuations. Moreover, Fig. 2 indicates that the cluster size of our simulations is sufficient to exhaust the self-energy of an individual chain.

Let us now turn to the case of spin-polarized systems. The fact that quasi-1D systems would favor the FFLO state in comparison to 3D systems was first suggested based on mean-field studies of a system of coupled 1D tubes [7]. The same qualitative conclusion was reached in [8] using effective field theory and treating the intertube coupling as a perturbation. On the other hand, real-space DMFT studies of coupled chains [9, 10] suggested

rather than the FFLO state is important in the entire dimensional crossover from quasi-1D to 3D lattices. One reason for differing predictions can be that the stabilization of FFLO in lattices due to nesting [11] is stronger for coupled chains than coupled tubes. Another possibility is a different treatment of quantum fluctuations. While the FFLO signatures have been absent in experiments on spin-polarized Fermi gases in continuum [28, 29], experiments in 1D tubes [30] are consistent with its possible existence.

Now, considering the large effect of the quantum fluctuations on the BCS transition, one might anticipate that the FFLO state which involves a delicate spatial symmetry breaking would be totally destroyed by the non-local quantum fluctuations. Here we show that, in fact, the FFLO state survives even in the presence of non-local quantum fluctuations, as shown in Fig. 1(b). The qualitative trend is similar to the BCS transition; the critical temperature of the FFLO phase decreases when the interchain hopping is reduced. At  $t_{\perp} = 0.2$  we find that the critical temperature of FFLO in the cluster model is lowered by a factor of 0.67 in comparison to the single-site approximation, while for the BCS critical temperature the corresponding ratio would be 0.74. At the critical temperatures reported in Fig. 1(b) the polarization of the system varies from  $P = 3\%$  at  $t_{\perp} = 0.2$  to  $P = 5\%$  at  $t_{\perp} = 0.3$  in the cluster simulations, whereas in the case of single-site DMFT we find a polarization of  $P = 6\%$  in the same range. Below  $t_{\perp} = 0.2$  we cannot reach the FFLO phase in our simulations as we are limited by the scaling of the computational cost.

Throughout the data, we find  $\Delta_j$  in FFLO state an approximately sinusoidal function. Moreover, we find that the oscillating order parameter is accompanied by a spatial modulation of the density with half the period of the order parameter, as demonstrated in Fig. 3(a). This agrees with the standard characterization of the FFLO state. In Fig. 3(b) we see the structure of the non-local part of the self-energy in the FFLO state. The similar, approximately sinusoidal, dependence on the position is found at all Matsubara frequencies, while the contribution of the non-local fluctuations is the largest at low frequencies, as expected from the analytical high frequency asymptotes. The fact that the cluster self-energy retains the same periodic structure at all frequencies, and furthermore, that the local part of the self-energy is dominant is suggesting that FFLO character of the many-body state is robust and experimentally discernible from a polarized superfluid by probes or imaging techniques sensitive to density modulations.

There is an additional point to be made about the convergence with cluster size in the spin-polarized case. In our simulations, we do not find the FFLO phase at cluster sizes below  $N_c \approx 30$ . The likely reason here is that the lowest possible non-zero pairing momentum,  $\mathbf{q} = 2\pi/N_c$ , leads to a too large increase in the kinetic energy of the

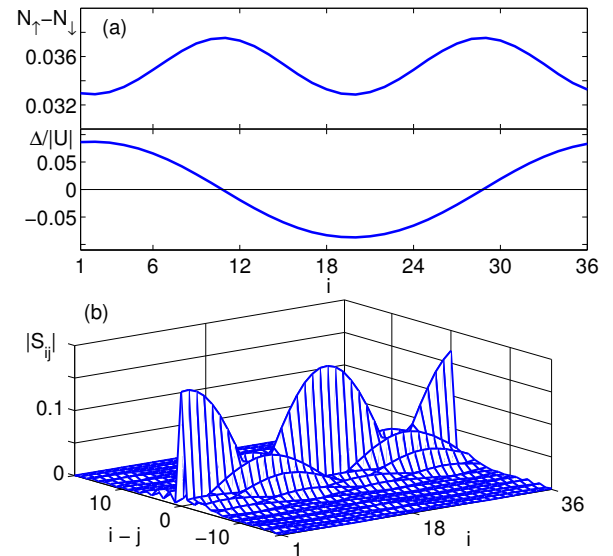


FIG. 3: The FFLO state at  $t_{\perp} = 0.25$ . Here, the temperature is  $T = 0.05$  and the polarization  $P = 0.035$ . (a) The density difference  $N_{\uparrow} - N_{\downarrow}$  and the order parameter  $\Delta$  as a function of the cluster site  $i$ . In our results, the translation invariance of the system is spontaneously broken and in a particular simulation in the FFLO regime e.g. the minima of the order parameter and density may fall on any given lattice site. (b) The absolute value of the anomalous part of the self-energy,  $S_{ij}(i\omega_n)$ , plotted as a function of the cluster site  $i$  and the distance  $i-j$  to the site  $j$  for the lowest Matsubara frequency.

Cooper pairs at  $N_c \lesssim 30$ . In other words, the FFLO transition is in essence orbitally limited in small clusters. Finally, it is interesting to speculate, if the non-local quantum fluctuations can in fact be favorable for the spatial symmetry breaking of the FFLO state by destabilizing the spatially uniform BCS state. The data at  $t_{\perp} = 0.3$  of Fig. 1(b) does in fact suggest a scenario along these lines. However, drawing this conclusion fully would require a further analysis of the role of the interchain quantum fluctuations on the FFLO state, and is beyond the scope of the present work.

In summary, we have shown that non-local quantum fluctuations play a crucial role in the low temperature properties of the attractive Hubbard model and affect heavily the fermionic superfluidity. Still, we find that even the exotic FFLO superfluid with broken translation invariance can endure the effect of the fluctuations, and possibly even compete better with the uniform polarized superfluid state because of the fluctuations. Our results suggest that the build-up of non-local quantum fluctuations can be studied in a systematic way in experiments on ultracold atoms in anisotropic optical lattices.

This work was supported by the Academy of Finland through its Centers of Excellence Programme (2012-2017) and under Projects No. 139514, No. 141039, No. 263347, No. 251748, No. 272490 and No. 135000, and by the European Research Council (ERC-

2013-AdG-340748-CODE and ERC-2011-AdG 290464-SIMCOFE). M.O.J.H. acknowledges support from the KAUTE-foundation. This research is supported in part by GIST college's 2013-2014 GUP research fund. Computing resources were provided by CSC—the Finnish IT Centre for Science and the Triton cluster at Aalto University.

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